3.4.2 Control boxes

CHANGE: When the CHANGE box is activated by clicking the mouse with the cursor within the CHANGE box boundaries, any parameter value may be changed simply by moving the cursor to the parameter position, clicking the mouse and entering the new value from the keyboard in response to the NCEMSS prompt. To leave CHANGE mode, deactivate the CHANGE box by clicking the mouse with the cursor once again positioned over the CHANGE box.

RUN: Activating the RUN box will cause NCEMSS to run an image simulation for the current values of the parameters shown in the PARAMETER menu. NCEMSS will automatically run the least required computation, starting with the PHSGRT program only if a structure parameter has been changed since the last run of this data, and starting with the IMAGE program if the only change has been in the electron microscope imaging parameters.

SHOW BASIS: This box will cause NCEMSS to display the BASIS menu, a list of the atom positions making up the basis (page 22).

SHOW ATOMS: this box will cause NCEMSS to display the ATOM-LIST menu, a list of all the atom positions in the unit cell (page 26).

PHSGRT: Activating the PHSGRT control box will run the PHSGRT sub-program for the current parameter values.

MSLICE: Activating the MSLICE control box will run the MSLICE sub-program for the current parameter values.

IMAGE: Activating the IMAGE control box will run the IMAGE sub-program for the current parameter values.

AMPLIT: Activating the AMPLIT control box will open up a plotting window (page 34), and ask the user which of the stored diffracted beam amplitudes to plot (assuming that some diffracted beams were stored by specifying their indices before the MSLICE was run).

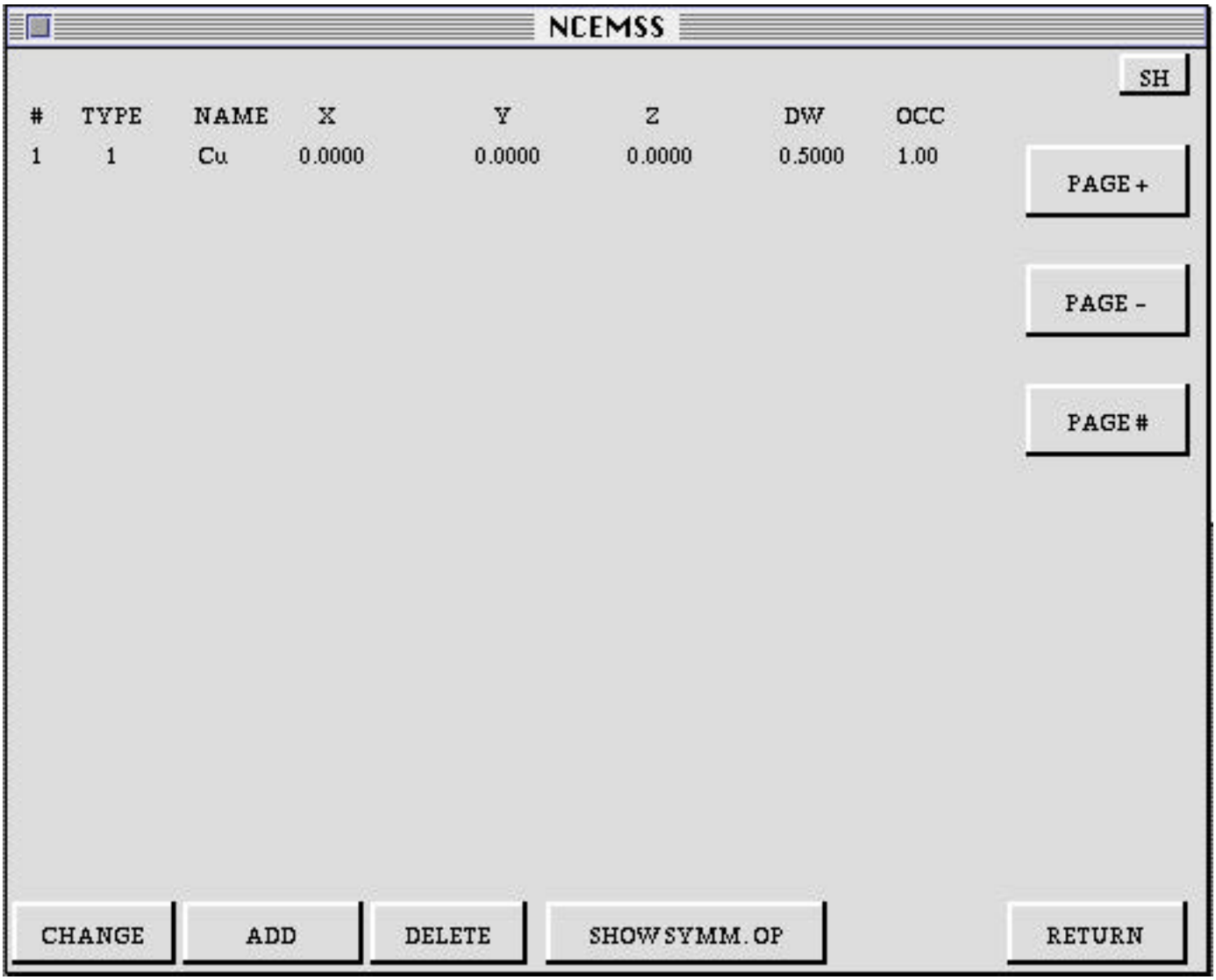
DISPLAY: This control box is used to activate the IMAGE-DISPLAY menu (page 38) for writing images to the display screen.

VIEW FILE: Activating this control box causes NCEMSS to ask which print file to display, then to display it.

CTF: Activating this control box produces a linear-image Contrast Transfer Function under the imaging conditions specified by the current parameter values (page 36).

RETURN: Return to previous FILE-LIST menu.

he BASIS Menu



3.5 The BASIS menu

The BASIS menu shows a list of the atom positions making up the basis; when operated upon by the symmetry operators, the basisyields the full set of unit cell atom positions. The BASIS menu displays the atom positions, showing the chemical symbol (NAME) for each atom, its fractional coordinates (X,Y,Z), the Debye-Waller factor, and the site occupancy. Subsequent pages of long lists can be viewed with the three right-hand control boxes.

CHANGE: The value of any parameter can be changed by activating the CHANGE box, then moving the cursor to the parameter position, clicking the mouse and entering the replacement value.

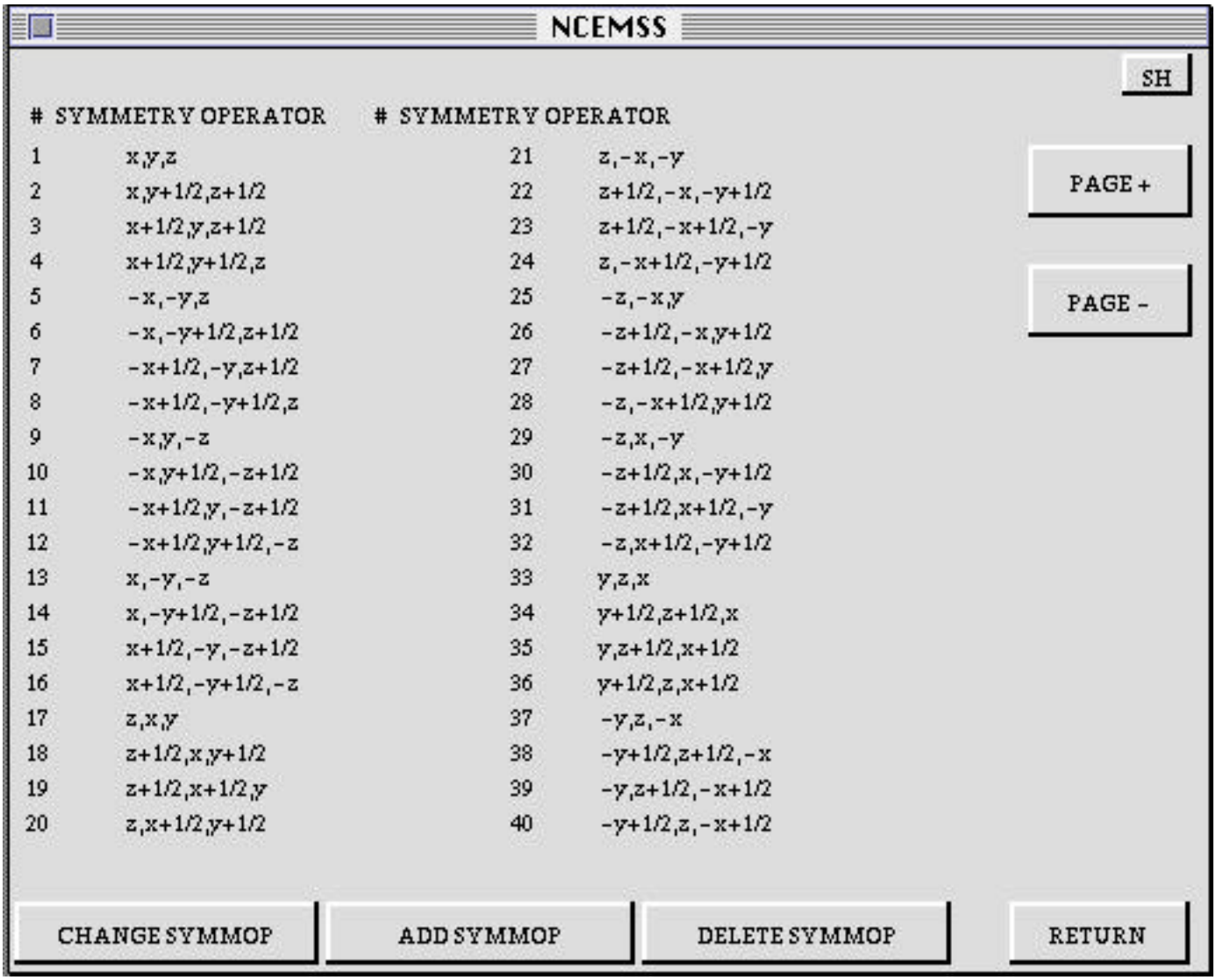
ADD: Additional atom positions may be added by activating the ADD box and entering parameter values in response to prompts.

DELETE: Activating the DELETE box, then moving the cursor to the appropriate line, will delete the line.

SHOW SYMM. OP: A list of the symmetry operators may be obtained by activating this control box in order to bring up the SYMM-OP menu (page 24).

RETURN: Return to previous MAIN menu.

The SYMMTRY-OPERATOR Menu



#	SYMMETRY OPERATOR	#	SYMMETRY OPERATOR
1	x,y,z	21	z,-x,-y
2	x,y+1/2,z+1/2	22	z+1/2,-x,-y+1/2
3	x+1/2,y,z+1/2	23	z+1/2,-x+1/2,-y
4	x+1/2,y+1/2,z	24	z,-x+1/2,-y+1/2
5	-x,-y,z	25	-z,-x,y
6	-x,-y+1/2,z+1/2	26	-z+1/2,-x,y+1/2
7	-x+1/2,-y,z+1/2	27	-z+1/2,-x+1/2,y
8	-x+1/2,-y+1/2,z	28	-z,-x+1/2,y+1/2
9	-x,y,-z	29	-z,x,-y
10	-x,y+1/2,-z+1/2	30	-z+1/2,x,-y+1/2
11	-x+1/2,y,-z+1/2	31	-z+1/2,x+1/2,-y
12	-x+1/2,y+1/2,-z	32	-z,x+1/2,-y+1/2
13	x,-y,-z	33	y,z,x
14	x,-y+1/2,-z+1/2	34	y+1/2,z+1/2,x
15	x+1/2,-y,-z+1/2	35	y,z+1/2,x+1/2
16	x+1/2,-y+1/2,-z	36	y+1/2,z,x+1/2
17	z,x,y	37	-y,z,-x
18	z+1/2,x,y+1/2	38	-y+1/2,z+1/2,-x
19	z+1/2,x+1/2,y	39	-y,z+1/2,-x+1/2
20	z,x+1/2,y+1/2	40	-y+1/2,z,-x+1/2

3.6 The SYMM-OP menu

The SYMM-OP menu shows a list of the symmetry operators generated by the chosen space group (or input by the user when a space group number of zero is entered in the MAIN menu - see page 20). The right-hand control boxes are used to page through long lists of symmetry operators.

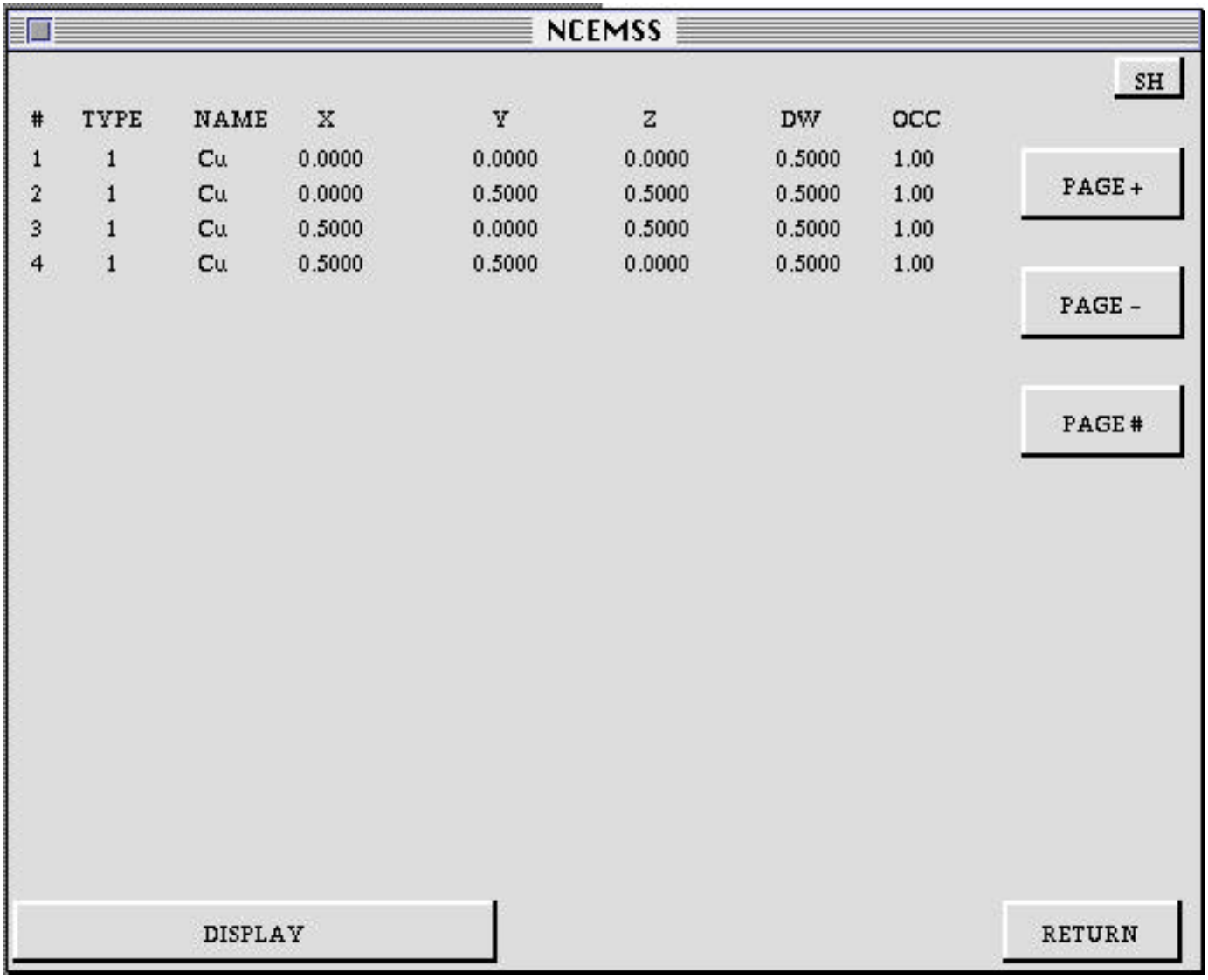
CHANGE: Any operator may be replaced by activating the CHANGE box, clicking the mouse over the appropriate line, and entering the new operator.

ADD SYMMOP: Activating this control box enables the user to add a new operator to the list.

DELETE SYMMOP: Activating this box, then placing the cursor over any operator and clicking the mouse, will delete that operator.

RETURN: Return to previous BASIS menu.

The Atom List Menu



3.7 The ATOM-LIST menu

The ATOM-LIST menu shows a list of the atom positions making up the unit cell. The list displays the atom positions one per line, showing the chemical symbol (NAME) for each atom, its fractional coordinates (X,Y,Z), the Debye-Waller factor (DW), and the site occupancy (OCC). Subsequent pages of long lists of atom position parameters can be viewed with the three right-hand control boxes.

BUILD CELL (not implemented on Unix Versions): Activating the BUILD control box brings up the BUILD menu (page 28) with the facility of generating defect cells.

DISPLAY: Activating this control box brings up the ATOM-DISPLAY menu (page 30), for the purpose of drawing an atom model of the current structure (page 32).

RETURN: Return to previous MAIN menu.

3.8 The BUILD menu

The BUILD menu is used to create defect cells visually with the aid of the cursor. The menu has a right-hand column of control buttons, activated in the usual way.

INCR_X: This button is used to increment the unit cell in the x direction. The INCR_Y button does the same in the y direction. When the INCR_X button is activated, NCEMSS will ask for the additional number of repeats to be input from the keyboard. Note that the total length of the new cell in the x-direction will be the original length plus the number of increments specified.

DISPLAY: This control box is used to display the current defect cell, and should be used on entering the menu, and after each change made to the defect cell.

INSERT: To insert an atom, activate this box and move the cursor to the required position. Note the changes in the fractional coordinates displayed in the bottom line of the menu as the cursor is moved. NCEMSS will prompt for parameter values.

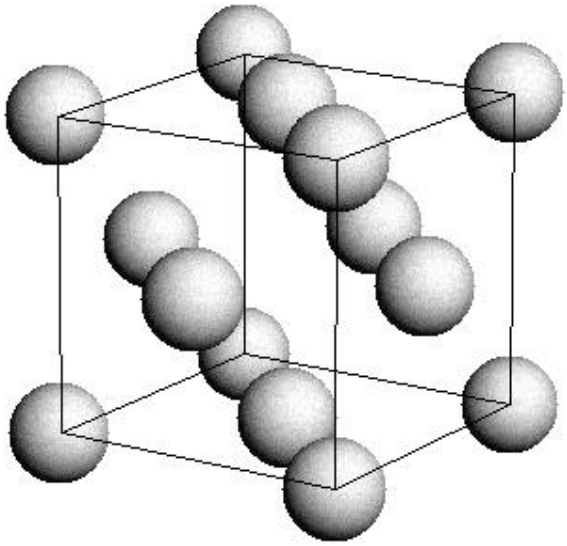
REMOVE: To remove an atom, activate this box and move the cursor to the appropriate atom, then click the mouse.

MOVE: To move an atom, activate this box, move the cursor to an atom position, click the mouse, move the mouse to the new position (note the fractional coordinates), and click again.

CHANGE: To change the atomic number of an atom, activate this box, and click the mouse at the atom position.

RETURN: Return to previous ATOM-LIST menu.

The ATOM-DISPLAY Menu



NCEMSS

SH

#	TYPE	NAME	X	Y	Z	DW	OCC
1	1	Cu	0.0000	0.0000	0.0000	0.5000	1.00
2	1	Cu	0.0000	0.5000	0.5000	0.5000	1.00
3	1	Cu	0.5000	0.0000	0.5000	0.5000	1.00
4	1	Cu	0.5000	0.5000	0.0000	0.5000	1.00

UNIT CELL | NEW UNIT CELL | UNIMPLEMENTED | RETURN